D-(-)-Mandelic acid 611-71-2 | DTXSID4046523

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 7.54e-01

Global applicability domain: Inside

Local applicability domain index: 6.34e-01

Confidence level: 8.91e-01

Nearest Neighbors from the Training Set

Image not found

Mandelic acid Measured: 0.62 Predicted: 7.54e-01 Image not found

Salicyl alcohol Measured: 0.73 Predicted: 7.49e-01 Image not found

3-Hydroxybenzyl alcohol

Measured: 0.49 Predicted: 6.45e-01